New World Vistas: New Models of Computation
Lattice Based Quantum Computation

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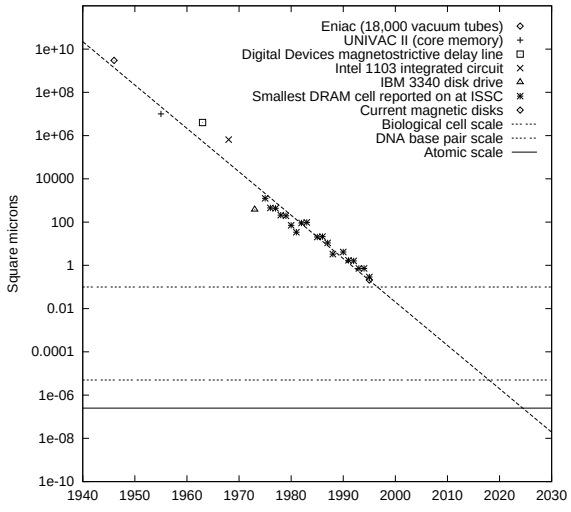

Figure 1: Exponential reduction in areal size of a bit for the last fifty years since the 1946 Eniac computer.

1 Planned Research

I propose to consider the feasibility of implementing a quantum lattice-gas dynamics based on quantum computing ideas and to explore the practicality of building a quantum computer, a question first posed by Richard Feynman over a decade ago [1].

It is likely, within our generation, nanometer scale computing will prevail as a standard computing technology. Fiqure 1 is a log-linear plot of data for the areal size of a bit over the last fifty years (from 18,000 bits in the 1946 Eniac computer to about 10^{11} in today's biggest parallel supercomputer). It is clear there has been an exponential reduction in bit size with its linear dimension halving approximately every 18 months. It appears a bit's size is heading towards the atom's size, and if the trend indicated in figure 1 continues, atomic densities will be achieved perhaps within two decades from now.

There are several important issues in nanoscale computing. While it may be possible to do classical computing at the nanoscale where bits are Boolean and have a definite value of either 0 or 1 [1], there exists a more compelling possibility, recently termed *quantum computing*, where spin-$\frac{1}{2}$ quantum objects represent the smallest unit of information, the quantum bit or "qubits". The qubit can be in a superposition of the Boolean states $\mid 0\rangle$ and $\mid 1\rangle$. If one measures the value of the qubit, binary values are observed corresponding to either the square of the probability amplitude of it being in the ground state, $|0\rangle$, or the square of the probability amplitude of it being in the excited state, $|1\rangle$. Of course, the probability of these classical outcomes add to unity: $\langle 0|0\rangle + \langle 1|1\rangle = 1$.

It is well known that lattice gases model kinetic processes for a large number of particles in a fine-grained parallel manner; in the macroscopic limit Navier-Stokes hydrodynamics emerges. Furthermore, lattice gases exhibit multiphase fluid behavior such as liquid-gas phase separation by spinoidal decomposition [10, 9, 7]. I propose to explore a generalization of the lattice gas idea. Consider the following quantum lattice gas microscopic transport equation[2]

$$\mid \psi(x_i + \varepsilon e_i, t + \varepsilon^2)\rangle = \mid \psi(x_i, t)\rangle + \hat{J} \mid \psi(x_i, t)\rangle, \quad (1)$$

where the lattice directions are denoted by the vectors $\hat{e}$. Require the evolution operator $\hat{1}+\hat{J}$ be unitary. The wave function $\mid \psi\rangle$ is a vector comprised of qubits. In

*My current classical lattice gas research for complex computational fluid dynamics is supported by Phillips Laboratory and the Air Force Office of Scientific Research under the Mathematical and Computational Sciences initiative task No. 2304CP.

[1] This kind of computing may best be termed *atomic-scale classical computing*.

[2] I am using diffusive ordering where $\delta t \sim \delta x^2 \sim \varepsilon^2$.

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the case of one-dimensions treated here for simplicity, there are two qubit per site, ψ_1 and ψ_2, corresponding to the positive and negative directions respectively, i.e. $\mid \psi\rangle = (\psi_1, \psi_2)$. Taylor expanding the L.H.S. of (1) gives the associated partial differential equation, to second order in ε,

$$\hat{J} \mid \psi(x,t)\rangle = \left(\epsilon C\partial_x + \frac{\varepsilon^2}{2}C^2\partial_x^2 + \varepsilon^2\partial_t\right) \mid \psi(x,t)\rangle. \tag{2}$$

C is a diagonal matrix whose components are those of the lattice vectors of the discrete space ($C_i^{\alpha\beta} = \delta_{\alpha\beta}e_{\alpha i}$). Substituting the wave amplitude

$$\mid \psi\rangle = \mid \psi^{(0)}\rangle + \varepsilon \mid \psi^{(1)}\rangle + \mathcal{O}(\varepsilon^2), \tag{3}$$

expanded in ε, into (2) and equating terms of similar order in ε gives the following equations[3]

$$\hat{J} \mid \psi^{(1)}\rangle = C\partial_x \mid \psi^{(0)}\rangle \tag{4}$$

$$\partial_t \mid \psi^{(0)}\rangle = -C\partial_x \mid \psi^{(1)}\rangle - \frac{1}{2}C^2\partial_x^2 \mid \psi^{(0)}\rangle. \tag{5}$$

(4) can be inverted to solve for the first order correction to wave function, $\mid \psi^{(1)}\rangle$. Substituting this into (5), a parabolic equation for $\mid \psi^{(0)}\rangle$ emerges

$$\partial_t \mid \psi^{(0)}\rangle = -C\left(\hat{J}^{-1} + \frac{1}{2}\right)C\partial_x^2 \mid \psi^{(0)}\rangle. \tag{6}$$

Now choosing the collision operator to be

$$\hat{J} = -\frac{2}{1+\frac{\hbar^2}{m^2}}\begin{pmatrix} 1 & i\frac{\hbar}{m} \\ i\frac{\hbar}{m} & 1 \end{pmatrix}, \tag{7}$$

(6) becomes the Schrödinger equation of a nonrelativistic quantum particle

$$i\hbar\partial_t\Psi = -\frac{\hbar^2}{2m}\partial_x^2\Psi, \tag{8}$$

where $\Psi = \psi_1 + \psi_2$. The "density" of qubits at a site, $\psi_1 + \psi_2$, obeys the Schrödinger equation (8). Therefore, it is possible to recover the Schrödinger equation from a quantum lattice gas, in analogy to the well known recovery of the Navier-Stokes equation from a classical lattice gas. It is straightforward to generalize this approach to n-dimensions and to the many-particle Schrödinger equation. This algorithm is naturally suited for a quantum computer, and can be implemented in terms of a few simple local unitary operations on a lattice of quantum bits.

[3] At zeroth order the operator $\hat{J}$ does not affect $\mid \psi^{(0)}\rangle$ since this is the equilibrium state.

2 Relevancy

Quantum mechanical systems of many interacting particles are notoriously difficult to simulate on classical computers. Even for systems of discrete spins, each of which may have only two possible states, the dimension of the Hilbert space of the entire system is exponential in the number of particles present. Since all first-principles methods of simulating such a system must follow the dynamics of all the components of the state vector in the full Hilbert space, they have a computational complexity that is exponential in the number of spins present.

In 1982 Feynman conjectured that it would be easier to simulate many-body quantum mechanical systems using other quantum mechanical systems, rather than using classical computers. This conjecture gave rise to the field of *quantum computation*. Until recently there were no specific algorithms known for implementing such a simulation in practice. In this project, I will explore a very simple quantum computational paradigm for the simulation of the many-particle Schrödinger equation in n-dimensions. Because all operations in these algorithms are local, they are easily implemented on parallel computers, which are often optimized for local operations and nearest-neighbor communication on a grid. However, in spite of this direct and immediate possible application, these ideas will assume their most powerful manifestation on a quantum computer, where they will make possible quantum many-body calculations that would otherwise require geological time scales to complete.

In either atomic-scale classical computing or quantum computing, one is restricted to reversible algorithms for reasons of avoiding heat production and the unitarity of quantum evolution. With nanoscale devices, heat dissipation is a fatal problem, one must avoid producing heat at all costs. Reversible logic achieves this. Since information is exactly preserved in a reversible algorithm, the Gibbs entropy, S, is constant throughout the course of the calculation ($dS = 0$), consequently since

$$dQ = TdS = 0, \tag{9}$$

no heat is produced. Furthermore, since all dynamics at the nanoscale is governed by the Schröedinger wave equation, where the Hamiltonian, H, is hermitian, the evolution operator

$$\hat{U} = e^{-i\hat{H}t} \tag{10}$$

is unitary, and hence its quantum evolution is invertible. The consequence of this to computing is that the

underlying quantum device itself would undergo reversible evolution. Conversely, for any reversible computation, one can describe the algorithm by permutations on the state data, for which there corresponds a unitary evolution (lattice gases are the prototypical example of this kind of algorithm). For any reversible algorithm chosen, the task is to map the computational "Hamiltonian" of the algorithm on to the physical Hamiltonian of the nanoscale device in question. Since microscopic physics is reversible, microscopic algorithms must be too. So a crucial issue in this regard is finding what are some useful reversible algorithms for physical modeling. Once these algorithms are found, the question of actually constructing a nanoscale device to implement these algorithms is somewhat more reasonable and more worth answering.

Nanoscale computing ofters unprecented parallelism. The notion of having information stored at atomic scales allows us to contemplate densities so high that any computation would necessarily have to be local, involving only nearby neighbors, and consequently would be ultimately fine-grained. So the issue of parallelism here involves coming up with a reasonable strategy of clocking such a large collection of bits.

Beyond this, in quantum computing, one tries to use a superposition of states as a practical means of parallel computing. This is termed *quantum parallelism*. For example, Shor's showed that factoring can in principle be done exponentially faster on a "quantum computer" than on a classical computer (the problem is NP-complete) by superposing all potential factors in the quantum computer's wave function and choosing an appropriate unitary evolution where wrong factors interfere destructively while correct factors interfere constructively [5]. In this way a massively parallel search is accomplished in the time a of single evolution of the quantum computer. So quantum computing relies on having interference of a collection of qubits occurring in a controlled fashioned to achieve unprecented parallelism not available in classical computing.

Qubits will likely be spin-$\frac{1}{2}$ objects. For example, two energy-level states in a solid-state quantum well or perhaps the spin of an electron localized in a laser controlled artificial quantum chain or in a long polymer molecular. Light might be used to initialize the spin states of the qubits (writing), and then after the qubits have interfered in some computing cycle, they might also be clocked by a sequence of light pulses; light might then likewise be used to measure the resulting spin states of the qubits (reading) [2]. (This kind of controlled light-and-matter interaction is well know in nuclear-magnetic-resonance experiments where pi-pulses are used to tip nuclear spins.) The most difficult issue for quantum computing is isolating the qubits from the surrounding environment. Since interference effects are essential for the computation, any coupling with the environment destroys such effects. The tremendous difficulties of maintaining quantum coherence remains an open issue that must be resolved before a quantum computer could be built.

3 Researchers and Facilities

Research will be carried out in the DynamicsLab computing facility at Phillips Laboratory/GPAA, 29 Randolph Road, Hanscom AFB, Massachusetts. The DynamicsLab is a new center for advanced parallel computing, comprised of researchers from the MIT, Boston University, Los Alamos National Laboratory, and Lawrence Livermore National Laboratory.

- J. Yepez, Physicist, PL/GPAA, Hanscom AFB
- B. Boghosian, Research Professor, Center for Comp Sci, Boston U., PL/GPAA IPA
- X. Shan, Research Scientist, Los Alamos National Laboratory, PL/GPAA IPA

On site resources include: two prototype massively parallel computers, CAM-8, an SGI power challenge array, several SGI workstations, several Sun workstations, and optical data libraries. Currently have accounts on several parallel supercomputers: DoD's 896-node CM-5 at the Army High Performance Research Computing Center, DoE's 1024 CM-5 at Los Alamos National Laboratory, and Phillips Laboratory's 400-node SP-2 at Maui.

4 Justification

I've been pioneering the area of new models of computation for several years and have been leading a new basic research initiative task 2304CP since 1993 supported by the Air Force Office of Scientific Research, Mathematical and Computational Science Directorate, in complex computational fluid dynamics using lattice-gas methods requiring ultra fine-grained parallel computers [6, 8].

With Phillips Laboratory SBIR contracts, two designs for a billion site massively parallel lattice-gas

Figure 2: The PL/GPAA lattice gas machine CAM-8, eight module prototype, can evolve a D-dimensional cellular space with 128 million sites where each site has 16 bits of data with a site update rate of 200 million per second. Designed at the MIT Lab for Comp Sci.

computer have been completed. Currently the facility has two working prototypes of a lattice-gas machine, the CAM-8, one with 32 million sites and the other with 128 million sites [4, 3]. The CAM-8 machine constitutes a significant improvement in our understanding of how to efficiently and flexibly model and analyze large-scale discrete systems. The CAM-8 is a mesh-network multiprocessor optimized for the large-scale simulation of lattice gas models. A uniform n-dimensional space is divided up evenly among a 3-dimensional array of processing nodes. Taking advantage of the uniformity and predictability of lattice gas computations, all memory accesses and communication events are optimally ordered, pipelined and synchronized between processors.

Hanscom Field, Masschusetts, in the Concord/Lexington suburbs just our side the Boston area is an ideal location because of its proximity to the local universities and laboratories: MIT, Boston University, Lincoln Laboratory, and many industrial corporations involved in state-of-the-art computing architectures.

5 Programmatics

The proposed research project will begin in the beginning of the fiscal year 1997.

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TOTALS	150K	150K	150K	150K	150K

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